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Mechanism of the hydrolysis reactions of 1-hydroxysilatrane and 1-hydroxygermatrane, 2,2-dihydroxysilocane and 2,2-dihydroxygermocane

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Abstract

© 2016 Taylor & Francis Group, LLC.The mechanism of the hydrolysis reactions of 2,2-dihydroxysilocane, 2,2-dihydroxygermocane, 1-hydroxysilatrane, and 1-hydroxygermatrane was studied by the density functional theory method. According to the quantum chemical calculations, the reactions of hydrolysis for 2,2-dihydroxysilocane and 2,2-dihydroxygermocane are characterized by the lower values of activation energy than for 1-hydroxysilatrane and 1-hydroxygermatrane. The ring configurations of the hydrolysis products are stable due to the presence of transannular interaction N→X (X = Si, Ge) and intramolecular hydrogen bond in their molecules.

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Keywords

atranes, germocanes, quantum chemical calculations, reaction mechanism, Silocanes